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A Discontinuous Galerkin Method for Strain Gradient Plasticity

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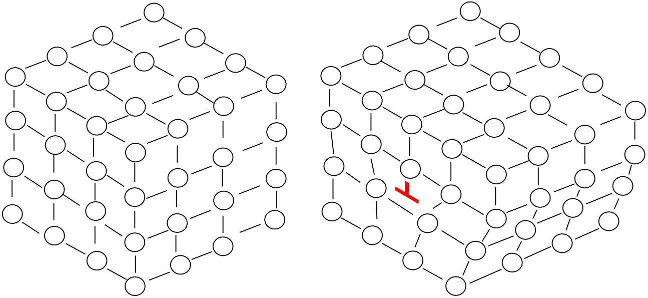
Outline

- Gradient Plasticity Model
- Discontinuous Galerkin (DG) Methods
- Results
- Conclusions

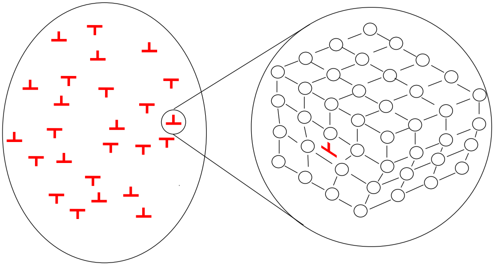
Physical Gradient Plasticity

- Objective: develop a particular version of gradient plasticity
- Physically reasonable
- Motivated by microstructural arguments
- Applicable polycrystalline materials (metals)



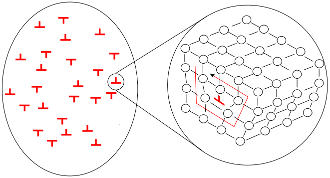
Physical Gradient Plasticity

- Plasticity caused by the motion of dislocations
- Dislocation account for permanent deformation and interactions induce hardening
- Dislocation density influences hardening



Burger's Tensor

- From Gurtin (2001, 2004, 2005)
- Decompose displacement gradient: $\nabla \boldsymbol{u} = \boldsymbol{H}^e + \boldsymbol{H}^p$
- A measure of the distortion in a material is $\boldsymbol{H}^p$
  - $\varepsilon^p = \mathrm{sym}\, \boldsymbol{H}^p$
- Use Stokes' theorem to obtain tensorial notion of incompatibility
- $\oint_{\partial S} \boldsymbol{H}^p \, \mathrm{d}\boldsymbol{X} = \int_S \underbrace{(\mathrm{curl}\, \boldsymbol{H}^p)}_{\boldsymbol{G}}{}^T \boldsymbol{n} \, \mathrm{d}A$
- $\boldsymbol{G}^T \boldsymbol{n}$ gives a measure of the Burger's vector, per unit area, for a plane with unit normal, $\boldsymbol{n}$



Incompatibility Based Gradient Plasticity

- Build up a theory Gurtin (2004)
- Variationally consistent, numerical methods inherit the variational basis, good for stability
- Introduce stress $\boldsymbol{T}^p$, and $\mathbb{S}$ conjugate to $\dot{\boldsymbol{H}}^p$ and $\dot{\boldsymbol{G}}$
- $\mathscr{W}_{int} = \int_\Omega \boldsymbol{\sigma} : \dot{\boldsymbol{H}}^e + \boldsymbol{T}^p : \dot{\boldsymbol{H}}^p + \mathbb{S} : \dot{\boldsymbol{G}} \, \mathrm{d}V$
- $\mathscr{W}_{ext} = \int_\Omega \boldsymbol{b} \cdot \dot{\boldsymbol{u}} \, \mathrm{d}V + \int_{\partial\Omega} \boldsymbol{S}(\boldsymbol{n}) : \dot{\boldsymbol{H}}^p \, \mathrm{d}S$
- Principal of virtual power, $\mathscr{W}_{int} = \mathscr{W}_{ext}$, yields two PDEs
  - Balance of momentum: $\operatorname{div} \boldsymbol{\sigma} + \boldsymbol{b} = \boldsymbol{0}$
  - Microforce balance: $\operatorname{dev} \boldsymbol{\sigma} = \boldsymbol{T}^p + (\operatorname{dev} \operatorname{curl} (\mathbb{S}^T))^T$

Constitutive Relations

- Derive constitutive equations for stresses from a free energy
  - $\Psi(\varepsilon^e, \boldsymbol{G}) = \frac{1}{2}\varepsilon^e : \mathbb{C} : \varepsilon^e + \frac{1}{2}k|\boldsymbol{G}|^2$
- Then the stresses take the forms
  - $\boldsymbol{\sigma} = \dfrac{\partial \Psi}{\partial \varepsilon^e} = \mathbb{C} : \varepsilon^e$
  - $\mathbb{S} = \dfrac{\partial \Psi}{\partial \boldsymbol{G}} = k\, \boldsymbol{G} = k \,\mathrm{curl}\, \boldsymbol{H}^p$
- Next the micro-stress is assumed as
  - $\boldsymbol{T}^p = \dfrac{\sigma_y}{d^p}\dot{\boldsymbol{H}}^p,\ d^p = \|\dot{\boldsymbol{H}}^p\|$
- Using the constitutive equations for the stresses, we can derive the flow rule from the microforce balance
  - $\mathrm{dev}\, \boldsymbol{\sigma} - \left(\mathrm{dev}\,\mathrm{curl}\left(k\,\mathrm{curl}\, \boldsymbol{H}^p\right)^T\right)^T = \dfrac{\sigma_y}{d^p}\dot{\boldsymbol{H}}^p$

Link to Classical Theory

- $\mathscr{W}_{int}$ and $\mathscr{W}_{ext}$ account for additional kinematics
- Another term is obtained
  - $(\operatorname{dev}\operatorname{curl}(\mathbb{S}^T))^T$
- The classical theory does not account for a dependence on $\mathbb{S}$
- In that case the microforce balance simplifies
  - $\operatorname{dev}\boldsymbol{\sigma} = \boldsymbol{T}^p = \frac{\sigma_y}{d^p}\dot{\boldsymbol{H}}^p$
- Under certain assumptions we recover classical theory
  - $\frac{\operatorname{dev}\boldsymbol{\sigma}}{\sigma_y} = \boldsymbol{n}, \quad d^p = \|\dot{\varepsilon}^p\| = \gamma$
  - $\dot{\varepsilon}^p = \gamma\boldsymbol{n}$

Classical Formulation

- Equilibrium
  - $\operatorname{div} \boldsymbol{\sigma} + \boldsymbol{b} = \boldsymbol{0}$

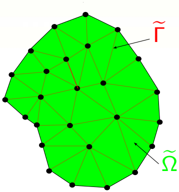
- Flow rule
  - $\operatorname{dev} \boldsymbol{\sigma} - \left(\operatorname{dev} \operatorname{curl} \left(k \operatorname{curl} \boldsymbol{H}^p \right)^T \right)^T = \frac{\sigma_y}{d^p} \dot{\boldsymbol{H}}^p$

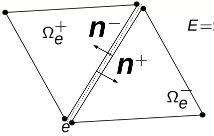
- Classical Weak Form
  - Find $\{\boldsymbol{u}, \boldsymbol{H}^p\} \in \mathscr{S} \times \mathscr{P} \subset H^1(\Omega) \times \operatorname{dev} H^1(\Omega)$ s.t.
    $\forall \{\boldsymbol{w}, \boldsymbol{V}\} \in \mathscr{V} \times \mathscr{Q} \subset H^1(\Omega) \times \operatorname{dev} H^1(\Omega)$:

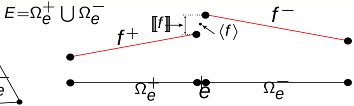
$$(\nabla \boldsymbol{w}, \boldsymbol{\sigma})_\Omega = (\boldsymbol{w}, \boldsymbol{b})_\Omega + (\boldsymbol{w}, \boldsymbol{t}(\boldsymbol{n}))_{\Gamma_t}$$

$$(\boldsymbol{V}, \boldsymbol{T}^p - \operatorname{dev} \boldsymbol{\sigma})_\Omega + (\operatorname{curl} \boldsymbol{V}, k \operatorname{curl} \boldsymbol{H}^p)_\Omega = (\boldsymbol{V}, \boldsymbol{S}(\boldsymbol{n}))_{\Gamma_s}$$

DG Machinery: Preliminaries







Average operator: $\langle \boldsymbol{f} \rangle = \frac{1}{2}(\boldsymbol{f}^+ + \boldsymbol{f}^-)$

Jump operator for a vector: $[\![\boldsymbol{u}(\boldsymbol{n})]\!] = \boldsymbol{u}^+ \cdot \boldsymbol{n}^+ + \boldsymbol{u}^- \cdot \boldsymbol{n}^-$

Jump operator for a tensor: $[\![\boldsymbol{\sigma}(\boldsymbol{n})]\!] = \boldsymbol{\sigma}^+ \boldsymbol{n}^+ + \boldsymbol{\sigma}^- \boldsymbol{n}^-$

Gradient plasticity jump: $[\![\boldsymbol{\sigma}(\boldsymbol{n}\times)]\!] = \boldsymbol{\sigma}^+(\boldsymbol{n}\times)^+ + \boldsymbol{\sigma}^-(\boldsymbol{n}\times)^-$

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DG Gradient Plasticity

- Consider the symmetric DG IP formulation for gradient plasticity
  - Find $\{\boldsymbol{u}^h, \boldsymbol{H}^{ph}\} \in \mathscr{S}^h \times \mathscr{P}^h \subset H^1(\Omega) \times \mathrm{dev}\, L^2(\Omega)$ s.t. $\forall \{\boldsymbol{w}^h, \boldsymbol{V}^h\} \in \mathscr{V}^h \times \mathscr{Q}^h \subset H^1(\Omega) \times \mathrm{dev}\, L^2(\Omega)$
  - $\underbrace{(\nabla \boldsymbol{w}^h, \boldsymbol{\sigma}^h)_\Omega = (\boldsymbol{w}^h, \boldsymbol{b})_\Omega,}_{\text{equilibrium}}$

$$\underbrace{(\boldsymbol{V}^h, \boldsymbol{T}^{ph} - \boldsymbol{\sigma}^h)_\Omega + (\mathrm{curl}\, \boldsymbol{V}^h, k\ \mathrm{curl}\, \boldsymbol{H}^{ph})_{\widetilde{\Omega}}}_{\text{domain}}$$

$$\underbrace{+([\![\boldsymbol{V}^h(\boldsymbol{n}\times)]\!], \langle (k\ \mathrm{curl}\, \boldsymbol{H}^{ph})^T \rangle)_{\widetilde{\Gamma}} + (\langle (k\ \mathrm{curl}\, \boldsymbol{V}^h)^T \rangle, [\![\boldsymbol{H}^{ph}(\boldsymbol{n}\times)]\!])_{\widetilde{\Gamma}}}_{\text{symmetric}}$$

$$\underbrace{+\frac{\alpha\, k}{h}([\![\boldsymbol{V}^h(\boldsymbol{n}\times)]\!], [\![\boldsymbol{H}^{ph}(\boldsymbol{n}\times)]\!])_{\widetilde{\Gamma}}}_{\text{penalty}}$$

$$= (\boldsymbol{V}^h, \boldsymbol{S}(\boldsymbol{n}))_{\Gamma_S}$$

DG Gradient Plasticity

- Euler-Lagrange equations for gradient plasticity

$$
\begin{aligned}
\left(\boldsymbol{w}^h, \operatorname{div} \boldsymbol{\sigma}^h + \boldsymbol{b}\right)_{\Omega} &= 0 \text{ (equilibrium)} \\
\left(\boldsymbol{V}^h, \boldsymbol{T}^{ph} - \boldsymbol{\sigma}^h + (\operatorname{curl}(k \operatorname{curl} \boldsymbol{H}^{ph})^T)^T\right)_{\widetilde{\Omega}} &= 0 \text{ (flow rule)} \\
\left(\langle (k \operatorname{curl} \boldsymbol{V}^h)^T \rangle, [\![\boldsymbol{H}^{ph} (\boldsymbol{n}\times)]\!]\right)_{\widetilde{\Gamma}} &= 0 \text{ (continuity of } \boldsymbol{H}^p(\boldsymbol{n}\times)\text{)} \\
\left(\langle \boldsymbol{V}^h \rangle, [\![(k \operatorname{curl} \boldsymbol{H}^{ph})^T (\boldsymbol{n}\times)]\!]\right)_{\widetilde{\Gamma}} &= 0 \text{ (continuity of } \mathbb{S}(\boldsymbol{n}\times)\text{)} \\
\left(\boldsymbol{V}^h, (\mathbb{S}^T (\boldsymbol{n}\times) - \boldsymbol{S}(\boldsymbol{n}))\right)_{\Gamma_S} &= 0 \text{ (micro-traction condition)}
\end{aligned}
$$

- Recall: $\mathbb{S} = k \operatorname{curl} \boldsymbol{H}^p$
- Note: important for analysis of method

Yield Condition

- Flow rule: $\boldsymbol{T}^p - \operatorname{dev}\boldsymbol{\sigma} + (\operatorname{dev}\operatorname{curl}(k\operatorname{curl}\boldsymbol{H}^p)^T)^T = 0$
- Approximate $\boldsymbol{\beta} \approx (\operatorname{dev}\operatorname{curl}(k\operatorname{curl}\boldsymbol{H}^p)^T)^T$
- Yield condition $f := \|\operatorname{dev}\boldsymbol{\sigma} - \boldsymbol{\beta}\| - \sqrt{\frac{2}{3}}\sigma_y$
- Two different methods of determining $\boldsymbol{\beta}$
  1. *lift-lift* evaluation of the back stress
     $(\boldsymbol{V}, \boldsymbol{S})_\Omega = -(\langle\boldsymbol{V}\rangle, [\![\boldsymbol{H}^p(\boldsymbol{n}\times)]\!])_{\tilde{\Gamma}}$
     $(\boldsymbol{V}, \boldsymbol{\beta})_\Omega = -(\langle\boldsymbol{V}\rangle, [\![\boldsymbol{S}(\boldsymbol{n}\times)]\!])_{\tilde{\Gamma}}$
  2. Exploitation of the flow rule
     $\boldsymbol{T}^p - \operatorname{dev}\boldsymbol{\sigma} + \boldsymbol{\beta} = \boldsymbol{0} \rightarrow \boldsymbol{\beta} = -\boldsymbol{T}^p + \operatorname{dev}\boldsymbol{\sigma}$
- Method 2) proved to be more robust

DG Gradient Plasticity Implementation

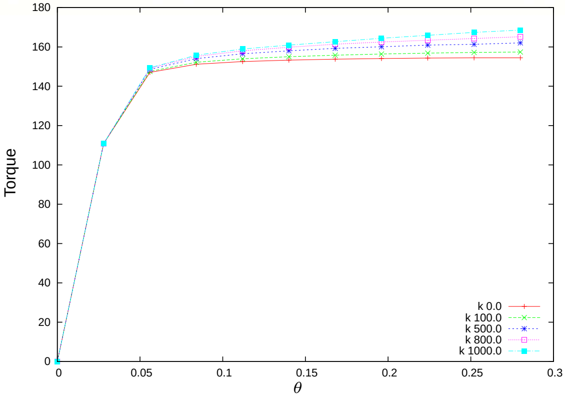
- Implementation of mixed method using symmetric DG IP formulation
- FEniCS: open source finite element code project
  - Variational form $\rightarrow$ generated C++ code $\rightarrow$ nonlinear solver
- Newton-Raphson iterative scheme for each PDE
- With the choice of $\boldsymbol{H}^p \in \mathscr{C}^{-1}$ the flow rule reduces
  - $(\boldsymbol{V}^h, \boldsymbol{T}^{ph} - \boldsymbol{\sigma}^h)_\Omega + \frac{\alpha k}{h}([\![\boldsymbol{V}^h(\boldsymbol{n}\times)]\!], [\![\boldsymbol{H}^{ph}(\boldsymbol{n}\times)]\!])_{\widetilde{\Gamma}} = 0$
- Backward Euler time integration

DG Gradient Plasticity Implementation

- Predictor stage: trial state
  - Evaluate yield condition f
  - IF: $f \geq 0$ Add current element to list of plastic elements
- Corrector stage: flow rule PDE
  - While plastic residual > TOL
  - Compute plastic quantities
  - Assemble plastic stiffness and plastic residual
  - Solve for $\boldsymbol{H}^p$
- Assemble and solve equilibrium equation for $\boldsymbol{u}$
- Check convergence and advance state $(\cdot)_{n+1} \rightarrow (\cdot)_n$, otherwise return to predictor

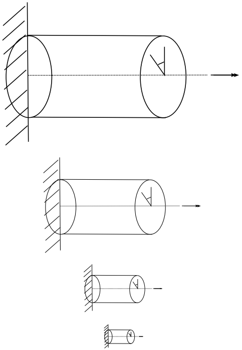
Gradient Hardening

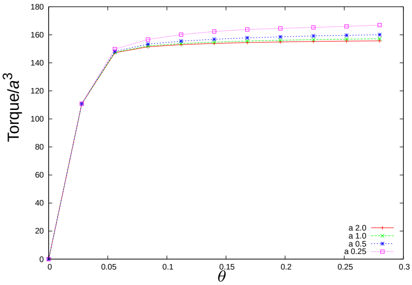
- Hardening increases with *k*



Size Effect

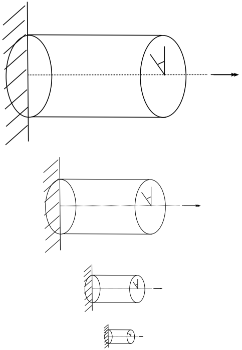
- Size effect for the torsion problem

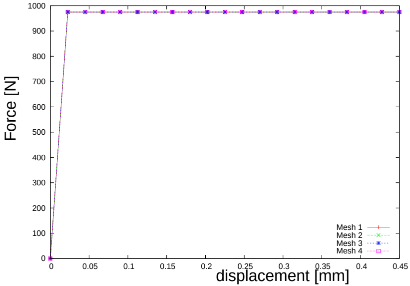




Size Effect

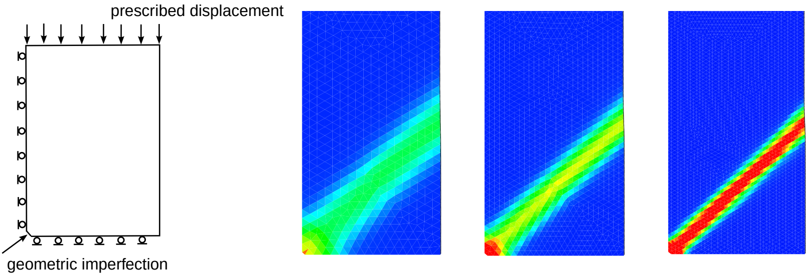
- No size effect for tension
- Representative of a macroscopic problem, gentle gradient





Localization

- Localization for classical softening



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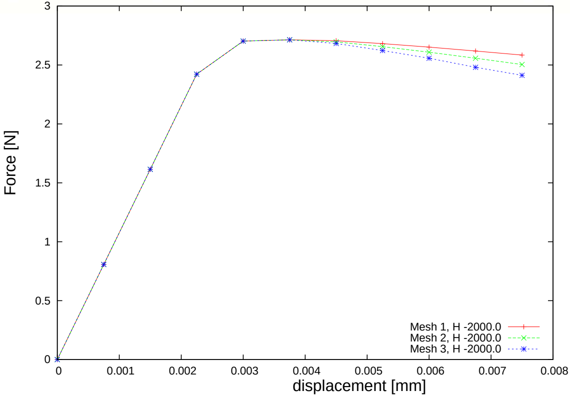
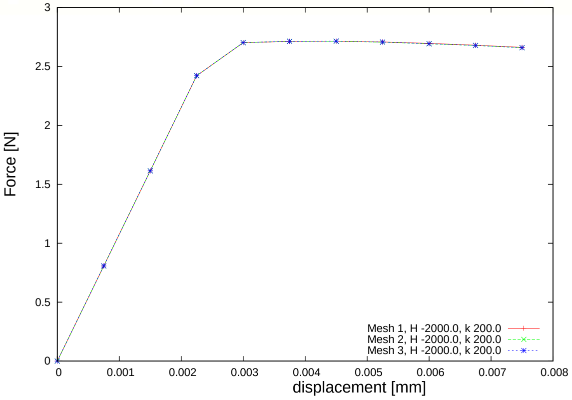


Localization

- Localization for classical softening with gradient hardening



Summary

- Summary
  - Developed physically reasonable, incompatibility-based strain gradient plasticity theory
  - Constructed variational formulation using concepts from DG methods
  - Implemented model into nonlinear finite element code
  - Predicted size effect for variable domain dimension to mimic that seen in plasticity at small scales
  - Regularized a softening induced localization
  - Investigated back-stress algorithms for gradient plasticity yield condition
  - Investigated integration algorithms for gradient plasticity